

An Improved FPRAS for Counting the Number of Hamiltonian Cycles in Dense Digraphs

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Abstract

We propose an improved algorithm for counting the number of Hamiltonian cycles in a directed graph. The basic idea of the method is sequential acceptance/rejection, which is successfully used in approximating the number of perfect matchings in dense bipartite graphs. As a consequence, a new ratio of the number of Hamiltonian cycles to the number of 1-factors is proposed. Based on this ratio, we prove that our algorithm runs in expected time of $O(n^{8.5})$ for dense problems. This improves the Markov Chain Monte Carlo method, the most powerful existing method, a factor of at least $n^{4.5}(\log n)^4$ in running time. This class of dense problems is shown to be nontrivial in counting, in the sense that they are #P-Complete.

Keywords: Hamiltonian Cycle, 1-factor, Counting, #P-Complete

1. Introduction

A Hamiltonian cycle is a closed directed path that visits each vertex once and only once. In this paper we use digraph to denote directed graph. Counting the number of Hamiltonian cycles is a very challenging problem and has applications, for example, in quantum physics [4]. Many intractable counting problems have been added to the Valiant's [20] list of #P-Complete, which is a natural correspondence of the concept NP-Complete for decision problems. Efficient approximating schemes called fully polynomial randomized approximation scheme(FPRAS) are naturally considered for the hard problems in counting. If M is the true value, a randomized

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algorithm is called an FPRAS if it takes polynomial time of size of inputs, ε^{-1} and $\log \delta^{-1}$ to obtain an output \tilde{M} . Here \tilde{M} is the approximation of M , satisfying

$$P((1 - \varepsilon)M \leq \tilde{M} \leq (1 + \varepsilon)M) \geq 1 - \delta.$$

Due to the fact that the decision problem of whether a graph contains a Hamiltonian cycle is NP-Complete, there would be no FPRAS for counting the Hamiltonian cycles for general graphs unless NP=RP. Thus the FPRAS for counting Hamiltonian cycles are only possible for special or restricted graphs, for example, elementary recursive algorithms [17] for random digraphs; Markov Chain Monte Carlo(MCMC) methods for dense *undirected* graphs[6], for some random digraphs[8] and random regular graphs[7].

Sequential acceptance/rejection method is introduced by Huber [9] for counting the number of the perfect matchings in a dense regular bipartite graph. Recently the regularity requirement is removed [10]. The primary tool used in the algorithm is the generalized Bregman's bound and the matrix scaling method.

The MCMC algorithm presented for random digraphs in [8] can be naturally extended to dense digraphs. This algorithm is based on sampling 1-factors of the digraphs and uses the self-reducing method[13] to approximate the counting. Recently Bezáková et. al. present an algorithm that approximates the number of 1-factors in $O(n^7(\log n)^4)$ expected time, via an accelerating simulated annealing technique[1].

The ratio of the number of 1-factors to the number of Hamiltonian cycles is established to be $O(n^{1+1/(2\alpha-3/2)})$ in this paper provided that the digraph is αn dense. Due to this ratio and Bezáková's results in [1], MCMC method[8] runs in an $O(n^{13}(\log n)^4)$ time when $\alpha \geq .85$. Moreover, counting the number of Hamiltonian cycles in such digraphs is shown to be still #P-Complete.

Our algorithm for counting Hamiltonian cycles is built on the acceptance/rejection algorithm in [10] while a different sequential sampling procedure is constructed to ensure that the approximating target is the number of Hamiltonian cycles.

One of the remarkable advantages of acceptance/rejection method is that it samples perfectly from a given set, which removes the sampling error when the MCMC method is adopted. Hence, our algorithm generates a weighted Hamiltonian cycle exactly according to its weight from the set of Hamiltonian cycles of a weighted digraph. In addition, this perfect sampling is only by-product when acceptance/rejection is used to approximate counting, which means the time used to sample a random Hamiltonian cycle can be used to approximate the number of the Hamiltonian cy-

cles without extra cost. The main result of this paper is summarized in the following.

Theorem M. *For any $\varepsilon, \delta \in (0, 1]$ and $\alpha \in (.75, 1]$, there exists a randomized approximation algorithm which provides an FPRAS for computing the number of Hamiltonian cycles of αn dense digraphs. The same algorithm approximates the number of Hamiltonian cycles by a factor in $[1 - \varepsilon, 1 + \varepsilon]$ with probability at least $1 - \delta$ and has the complexity $O(n^{2.5+.5/(2\alpha-1)+1/(2\alpha-1.5)}\varepsilon^{-2}\log(\delta^{-1}))$. In particular, when $\alpha \geq .85$, the running time is bounded by $O(n^{8.5})$.*

The remainder of the paper is structured as follows. In Section 2 some basic definitions, notations and lemmas are presented. In Section 3 we describe the algorithm in details. Section 4 contributes to the complexity of the algorithm and the hardness of counting. Further discussion and conclusion are proposed in Section 5.

2. Preliminaries

Consider a simple weighted digraph $G = (V, E)$ with the vertex set $V = \{1, \dots, n\}$ and the edge set E . Each edge $(i, j) \in E$ is endowed with a positive weight w_{ij} . Let $|S|$ denote the cardinality of any set S . The set of vertices pointing to i is denoted by $N^-(i, G) = \{j : (j, i) \in E\}$, and similarly that out of i by $N^+(i, G) = \{j : (i, j) \in E\}$. Indegrees and outdegrees of the vertex i are denoted by $\Delta^-(i) = |N^-(i, G)|$, $\Delta^+(i) = |N^+(i, G)|$ respectively. Let $\Delta(i) = \min(\Delta^-(i), \Delta^+(i))$ and $\Delta = \min_{i \in V} \Delta(i)$. G is called αn dense if $\Delta \geq \alpha n$ for an $\alpha > 0$ given. Let \oplus denote the symmetric difference of two sets and $\lfloor n \rfloor$ denote the maximum integer no more than n . A/B is used to denote the set by removing elements of B from the set A . With a little abuse of notation, $/$ also denote the quotient of two numbers. A Hamiltonian cycle in G is represented by

$$\mathcal{H} = (k_1, k_2, \dots, k_n, k_1),$$

where $\{k_1, k_2, \dots, k_n\}$ is a permutation of $\{1, \dots, n\}$ such that $(k_n, k_1) \in E$, and $(k_j, k_{j+1}) \in E$, $j = 1, \dots, n-1$. The length of a cycle or path is defined as the number of its edges that contains.

An 1-factor is defined as a spanning directed subgraph of G in which indegrees and outdegrees of each vertex are all one. An example of an 1-factor is a spanning union of vertex disjoint directed cycles. Obviously, a Hamiltonian cycle is a special 1-factor with only one cycle. The weight $W(F)$ of an 1-factor F with edge set

$\{e \in E\}_{e \in F}$ is defined as $W(F) = \prod_{e \in F} w_e$. The total weight $W(S)$ of the set S of 1-factors are defined as $W(S) = \sum_{F \in S} W(F)$. Let $W_F(G)$ and $W_H(G)$ denote the total weight of all the 1-factors and Hamiltonian cycles in G respectively. It is easy to see if $w_{ij} = 1$ for all $(i, j) \in E$, then $W_F(G)$ and $W_H(G)$ are the number of 1-factors and Hamiltonian cycles in G respectively.

Let A_G be the adjacent matrix associated with G where $A_G(i, j) = w_{ij}$ if $(i, j) \in E$ and $A_G(i, j) = 0$ otherwise. For an $n \times n$ matrix A , where n is the order of A , we use notation A_{ij} to denote the $(n-1) \times (n-1)$ matrix obtained from A by removing row i and column j . If there is no confusion, A'_{ij} or $(A_{ij})'$ denotes the $(n-1) \times (n-1)$ matrix obtained from A by, first permutating row i and row j and then removing row j and column j . Next we will define two quantities on the matrix A_G which are related to 1-factors and Hamiltonian cycles respectively.

Definition 1. The permanent of an $n \times n$ matrix $A = (A(i, j))_{n \times n}$ is

$$\text{per}(A) = \sum_{\sigma} \prod_{i=1}^n A(i, \sigma(i)),$$

where σ ranges over all the permutations of $\{1, \dots, n\}$.

Definition 2. The Hamilton of an $n \times n$ matrix $A = (A(i, j))_{n \times n}$ is defined as

$$\text{ham}(A) = \sum_{\{k_1, \dots, k_{n-1}\}} A(k_1, 1) A(k_2, k_1) \cdots A(k_{n-1}, k_{n-2}) A(1, k_{n-1}),$$

where $\{k_1, \dots, k_{n-1}\}$ ranges over all the permutations of $\{2, \dots, n\}$ when $n \geq 2$, and $\text{ham}(A) = A(1, 1)$, if $n = 1$.

By the definition of permanent and Hamilton, it is not difficult to see that $\text{per}(A) \geq \text{ham}(A)$ if the entries of A are all nonnegative. Suppose $A = A_G$. For any permutation (k_1, \dots, k_{n-1}) of $(2, \dots, n)$, $A_G(1, k_{n-1})$, $A_G(k_{n-1}, k_{n-2})$, \dots , $A_G(k_2, k_1)$, $A_G(k_1, 1)$ are the edge weight of the Hamiltonian cycle $(1, k_{n-1}, \dots, k_1, 1)$ in G if and only if they are all positive. Therefore, we have

$$W_H(G) = \text{ham}(A_G).$$

Note that the diagonal entries of A_G are all zero, and for any permutation σ over $\{1, 2, \dots, n\}$, $A(i, \sigma(i)) > 0$, $i = 1, \dots, n$ if and only if their corresponding edges in

G form an 1-factor of G . Hence

$$W_F(G) = \text{per}(A_G).$$

Next we present the Laplacian expansion formulas for the permanent and the Hamilton.

Lemma 3. *Let $A = (A(i, j))_{n \times n}$ be an $n \times n$ matrix. The permanent of empty matrix is set to be 1. Then*

$$\text{per}(A) = \sum_{i=1}^n A(i, 1) \text{per}(A_{i1}).$$

Lemma 4. *Let $A = (A(i, j))_{n \times n}$ be an $n \times n$ matrix, $n \geq 2$. Then*

$$\text{ham}(A) = \sum_{i=2}^n A(i, 1) \text{ham}(A'_{i1}).$$

For the permanent, this expansion is well known. For the Hamilton, the formula is very similar and [17] proposes a combinatorial proof when each edge weight of the digraph is one. Regarding its importance in our algorithm, a proof in terms of matrix is presented below. We emphasize Lemma 4 is crucial in the sequential sampling procedure which is different from the one used in [10], and ensures our algorithm to approximate the number of Hamiltonian cycles.

Proof of Lemma 4. We proceed to prove the lemma by induction on n , the order of the matrix.

The case $k = 2$ is trivial.

Suppose Lemma 4 holds for $k = n - 1$.

Consider $k = n$. Since

$$\text{ham}(A) = \sum_{i=2}^n A(i, 1) \sum_{\{k_2, \dots, k_{n-1}\}} A(k_2, i) A(k_3, k_2) \cdots A(k_{n-1}, k_{n-2}) A(1, k_{n-1}),$$

it is sufficient to show that

$$\text{ham}(A'_{i1}) = \sum_{\{k_2, \dots, k_{n-1}\}} A(k_2, i) \cdots A(k_{n-1}, k_{n-2}) A(1, k_{n-1}),$$

for $i = 2, \dots, n$, where $\{k_2, \dots, k_{n-1}\}$ goes over all the permutations of $\{2, \dots, n\}/i$. Considering the definition of A'_{i1} , the row $i-1$ of A'_{i1} is the first row of A except removing the first element, and

$$\begin{aligned} A'_{i1}(k_2 - 1, i - 1) &= A(k_2, i), \dots \dots, \\ A'_{i1}(k_{n-1} - 1, k_{n-2} - 1) &= A(k_{n-1}, k_{n-2}), \text{ and} \\ A'_{i1}(i - 1, k_{n-1} - 1) &= A(1, k_{n-1}). \end{aligned}$$

By the hypothesis of the induction, the order of A'_{i1} is $n-1$, then

$$\begin{aligned} \text{ham}(A'_{i1}) &= \sum_{\{k'_2, \dots, k'_{n-1}\}} A'_{i1}(k'_2, i - 1) \cdots A'_{i1}(k'_{n-1}, k'_{n-2}) A'_{i1}(i - 1, k'_{n-1}) \\ &= \sum_{\{k_2, \dots, k_{n-1}\}} A'_{i1}(k_2 - 1, i - 1) A'_{i1}(k_{n-1} - 1, k_{n-2} - 1) A'_{i1}(i - 1, k_{n-1} - 1) \\ &= \sum_{\{k_2, \dots, k_{n-1}\}} A(k_2, i) \cdots A(k_{n-1}, k_{n-2}) A(1, k_{n-1}), \end{aligned}$$

where $\{k'_2, \dots, k'_{n-1}\}$ and $\{k_2, \dots, k_{n-1}\}$ go over all the permutations of $\{1, \dots, n-1\}/\{i-1\}$ and $\{2, \dots, n\}/\{i\}$ respectively. This completes the proof of Lemma 4. \square

Hamiltonian Recovery Let $A = (A(i, j))_{n \times n}$ be an $n \times n$ positive matrix. The following procedure is applied to selecting elements from A (The first two steps are given explicitly). We call this procedure Selecting Hamiltonian Cycle(SHC for simplicity).

Step 1. Let $A^1 = A$. Choose a natural number $1 < j_1 \leq n$, denote $\pi(1) = j_1$ and select $A^1(\pi(1), 1)$.

Step 2. Let $A^2 = (A^1_{j_1 1})'$. Choose a natural number $1 < j_2 \leq n-1$, denote $\pi(2) = j_2$ and select $A^2(\pi(2), 1)$.

Similarly A^k , $\pi(k)$ and $A^k(\pi(k), 1)$, $1 \leq k \leq n-1$ can be obtained in Step k iteratively. Since A^n has only one entry, let $A^n = (A^{n-1}_{j_{n-1} 1})'$, $\pi(n) = j_n = 1$ and select $A^n(\pi(n), 1)$.

By Lemma 4, the set of selected elements $A^k(\pi(k), 1)$, $k = 1, \dots, n$, from the above procedure forms the edge weight of a Hamiltonian cycle in G if $A = A_G$. If $\pi(1), \pi(2), \dots, \pi(n)$ is given, we provide a simple algorithm to determine which Hamiltonian cycle in G is selected. This process is called Hamiltonian Recovery.

The input of the algorithm is $\pi = (\pi(1), \pi(2), \dots, \pi(n))$. We illustrate how to

recover an entry in A^2 if $\pi(1)$ is given. Let $A^2(i, j)$ be any entry in A^2 . Since $A^2 = (A^1_{\pi(1)1})'$ and recall the definition of $(A^1_{\pi(1)1})'$, which is obtained by, first permutating row $\pi(1)$ and the first row and then removing the first row and first column. Hence, if $i = \pi(1) - 1$ then $(1, j + 1)$ is the position where $A^2(i, j)$ lies of A^1 ; otherwise $(i + 1, j + 1)$ is the position where $A^2(i, j)$ lies of A^1 . Hence, if the vector $(\pi(1), \dots, \pi(k - 1))$ is given from the SHC procedure, the position of $A^k(\pi(k), 1)$ in A^1 can be found recursively by determining its position in A^{k-1} , then in A^{k-2} , and finally in A^1 . Since at each step of the SHC procedure an element is selected from the first column, $A^k(\pi(k), 1)$ must lie in column k of A^1 .

If $(1, k_1, \dots, k_{n-1}, 1)$ is the corresponding Hamiltonian cycle of $\pi = (\pi(1), \pi(2), \dots, \pi(n))$, then k_i can be obtained from k_{i+1} since the element $A(k_i, k_{i+1})$ is selected in Step k_{i+1} of the SHC procedure, or equivalently (k_i, k_{i+1}) is the position of $A^{k_{i+1}}(\pi(k_{i+1}), 1)$ in A , $i = 1, 2, \dots, n - 2$. Obviously, $k_{n-1} = \pi(1)$. By this simple procedure, it takes $O(n^2)$ time to recover all the positions of $A^k(\pi(k), 1)$, $1 \leq k \leq n$. We present the recovery algorithm explicitly.

Hamiltonian Recovery Algorithm

Input : The vector $(\pi(1), \pi(2), \dots, \pi(n))$.

Output : A Hamiltonian cycle $(1, k_1, \dots, k_{n-1}, 1)$.

Step 1: Set $k_{n-1} = \pi(1)$;

For $i = n - 2$ to 1

Set $a = \pi(k_{i+1})$;

For $j = k_{i+1}$ to 2

If $a = \pi(j - 1) - 1$; Set $a = 1$;

Else Set $a = a + 1$;

End;

Set $k_i = a$;

End;

Goto Step 2;

Step 2: Output $(1, k_1, \dots, k_{n-1}, 1)$.

For simplicity, let $HR(\pi)$ denote the output of the Hamiltonian Recovery Algorithm when the input is $\pi = (\pi(1), \pi(2), \dots, \pi(n))$.

3. Algorithms for Counting

One main tool in our algorithm is a generalized version of Bregman's bound for the permanent below, which generalized an inequality of Soul [19] and proved in [10]. For more application of other generalization of Bregman's bound for designing new algorithms or improving efficiency of algorithms, we refer to [14, 18]. Let

$$g(r) = \begin{cases} r + (1/2) \log r + e - 1, & r \geq 1 \\ 1 + (e - 1)r, & r \in [0, 1]. \end{cases}$$

Lemma 5. ([10]) *Let A be an $n \times n$ matrix with entries in $[0, 1]$. Denote $r(i)$ the sum of row i of A . Define $Br(A) = \prod_{i=1}^n (g(r(i))/e)$, then*

$$Br(A) \geq \sum_{i=1}^n A(i, 1) Br(A_{i1}).$$

In particular, by Lemma 3, $\text{per}(A) \leq Br(A)$.

Chernoff's bound is useful in our algorithm, and one form of that is given below [16].

Lemma 6. *Let x_1, x_2, \dots, x_t be identical independent distributed (i.i.d.) Bernoulli random variables with $P(x_1 = 1) = p$ and $P(x_1 = 0) = 1 - p$, $p > 0$, then for any $0 \leq \varepsilon \leq 2e - 1$,*

$$P\left(\left|\sum_{i=1}^t x_i - tp\right| > \varepsilon tp\right) \leq e^{-tp\varepsilon^2/4}.$$

For simplicity, in this section we only consider the digraph G with all edge weight equalling one. Hence the adjacent matrix A_G is a 0-1 matrix and $\text{ham}(A_G)$ is the number of Hamiltonian cycles in G . G is also restricted to be αn dense, $\alpha \geq .75$. It is known [2] that if G is $.5n$ dense, G must contain a Hamiltonian cycle and the proof can be easily modified to give an $O(n^2)$ algorithm to construct a Hamiltonian cycle. Hence $\text{ham}(A_G) \geq 1$. By the definition of Hamilton, if we change any zeros in A_G to $\gamma = (\varepsilon/3)((n-1)!)^{-1}$, $\text{ham}(A_G)$ increases by at most a factor of $1 + \varepsilon/3$.

Now we introduce the basic idea of acceptance/rejection method for the counting problem. Suppose S is a large set and each element in it with positive weight. The target is to approximate the total weight of all the elements in S . First select a

suitable large M such that $M > \sum_{b \in S} w(b)$. The main idea of acceptance/rejection method for approximation is to design a procedure to sample a random element x from the set S with the successful probability $P(x = a) = \frac{w(a)}{M}$, where $w(a)$ is the weight of $a \in S$, and failing probability $P(x \notin S) = 1 - \frac{\sum_{b \in S} w(b)}{M}$. At each time, if a random element a is successfully selected from S , we say acceptance or a is accepted, and if no element is selected from S , we say rejection. Hence, at each time the probability of acceptance is $\frac{\sum_{b \in S} w(b)}{M}$ and probability of rejection $1 - \frac{\sum_{b \in S} w(b)}{M}$. With some fundamental statistical knowledge, the total weight of S can be approximated by multiplying M and the ratio of acceptance over all the samplings. For our purpose, generalized Bregman's bound in Lemma 5 provides such a suitable large M , and self-reducing method for counting Hamiltonian cycles naturally proposes such a sampling procedure, which is sequential sampling procedure guaranteed by Lemma 4. For more details about sequential acceptance/rejection method, we refer to [10].

In order to make use of the generalized Bregman's bound in Lemma 5, before resuming the acceptance/rejection algorithm, we need to scale the matrix A_G to nearly be doubly stochastic and make each entry in $[0,1]$ [15]. Hence the algorithm has two phases.

Sub Algorithm I. Scale Matrix

Input : A_G, ε

Output : X, Y, Z, C

Step 1: Set $A_G(i, j) = (\varepsilon/3)((n-1)!)^{-1}$ if $A_G(i, j) = 0$ for all i, j , goto Step 2;

Step 2: Using matrix scaling to find diagonal matrix X, Y such that the row and column sums of $B = XA_GY$ in $(1 - (.1)n^{-2}, 1 + (.1)n^{-2})$, goto Step 3;

Step 3: Let Z be a diagonal matrix with $Z(i, i) = \min_j B(i, j)^{-1}$ for $i = 1, \dots, n$, goto Step 4;

Step 4: $C = ZB$.

After matrix scaling, matrix C satisfies the requirement of generalized Bregman's bound. Sequential acceptance/rejection method can be used to estimate $\text{ham}(C)$. Note that the matrix C is corresponding to a weighted digraph denoted by G_C .

Sub Algorithm II. Approximating Hamilton via Acceptance/Rejection

Input : $X, Y, Z, C, \varepsilon, \delta N$.

Output : $\mathcal{H}_1, \dots, \mathcal{H}_s; \widetilde{\text{ham}}(A_G)$ the estimator of $\text{ham}(A_G)$.

Step 5: Set $t = 4N(\varepsilon/2)^{-2} \log(\delta^{-1})$, $l = \prod_{i=1}^n (X(i, i)Y(i, i)Z(i, i))$, $D = C$, $k = 0$ and $s = 0$, goto Step 6;

Step 6: Set $r = \text{order of } D$;

If $r = 1$;

Set $p(1) = D/Br(D)$ and $p(0) = 1 - p(1)$;

Choose I from $\{0, 1\}$ according to $P(I = i) = p(i)$, $i = 0, 1$;

If $I > 0$; Set $\pi(n) = 1$, $s = s + 1$, $k = k + 1$ and $\mathcal{H}_s = HR(\pi)$;

If $k < t$; Set $D = C$, goto Step 6; Otherwise goto Step 7;

Else $I = 0$; Set $k = k + 1$;

If $k < t$; Set $D = C$, goto Step 6; Otherwise goto Step 7;

Else $r > 1$;

Set $p(i) = D(i, 1)Br(D'_{i1})/Br(D)$ for $i = 2, \dots, r$ and $p(0) = 1 - \sum_{i=2}^r p(i)$;

Choose I from $\{0, 2, 3, \dots, r\}$ according to $P(I = i) = p(i)$, $i = 0, 2, \dots, r$;

If $I > 0$; Set $\pi(n + 1 - r) = I$ and $D = D'_{I1}$, goto Step 6;

Else $I = 0$; Set $k = k + 1$

If $k < t$; Set $D = C$, goto Step 6; Otherwise goto Step 7;

Step 7: $\widetilde{\text{ham}}(A_G) = l^{-1}st^{-1}Br(C)$.

The procedure of sampling elements in Step 6 is the same as SHC procedure except selecting an element with certain probability or rejection when $I = 0$ is selected. The output \mathcal{H}_i , $1 \leq i \leq s$, is accepted by the algorithm.

Theorem 7. Let $\mathcal{H}_1, \dots, \mathcal{H}_s$ and $\widetilde{\text{ham}}(A_G)$ be the output of Sub Algorithm II. If we set $N = Br(C)/\text{ham}(C)$ in the same algorithm, and let H be a random variable recovered from a random π of Sub Algorithms II and S denote the set of all the possible accepted hamiltonian cycles, then

$$P(H = \mathcal{H}_1 | H \in S) = W(\mathcal{H}_1)/W_H(G_C)$$

and

$$P((1 - \varepsilon) \text{ham}(A_G) \leq \widetilde{\text{ham}}(A_G) \leq (1 + \varepsilon) \text{ham}(A_G)) \geq 1 - \delta.$$

Proof. First, we check $p(0) \geq 0$ at each level of Step 6, which guarantees the proceeding of the algorithm. By the definition of D'_{i1} and D_{i1} , obviously, $Br(D'_{i1}) =$

$Br(D_{i1})$. Using Lemma 5, it is easy to see

$$\begin{aligned} \sum_{i=2}^n D(i, 1) Br(D'_{i1}) &= \sum_{i=2}^n D(i, 1) Br(D_{i1}) \\ &\leq \sum_{i=1}^n D(i, 1) Br(D_{i1}) \\ &\leq Br(D). \end{aligned}$$

Hence $p(0) \geq 0$. Suppose $\mathcal{H}_1 = HR(j)$, $j = (j_1, \dots, j_n)$. Following the path in which \mathcal{H}_1 is selected, and using the notation in SHC procedure, then $C^{i+1} = (C_{j_i 1}^i)'$, $i = 1, \dots, n-1$ and $C^1 = C$, we have

$$P(\pi(k) = j_k) = \frac{C^k(j_k, 1) Br((C_{j_k 1}^k)')}{Br(C^k)},$$

where $k = 1, 2, \dots, n-1$ and $P(\pi(n) = j_n) = \frac{C^n(j_n, 1)}{Br(C^n)}$.

Since the selection at each level in Step 6 is independent of the other, the probability of selecting \mathcal{H}_1 is the telescoping product. Noting that $C^{i+1} = (C_{j_i 1}^i)'$, $i = 1, \dots, n-1$ and $C^1 = C$, then

$$P(H = \mathcal{H}_1) = P(\pi = j) = \prod_{k=1}^n P(\pi(k) = j_k) = \frac{\prod_{i=1}^n C^i(j_i, 1)}{Br(C)} = \frac{W(\mathcal{H}_1)}{Br(C)}.$$

Since each Hamiltonian cycle in G_C can be accepted with certain probability proportional to its weight, the acceptance set S is the set of all the Hamiltonian cycles in G_C . Then

$$P(H \in S) = \sum_{\mathcal{H} \in G_C} P(H = \mathcal{H}) = \frac{W_H(G_C)}{Br(C)}.$$

Hence,

$$P(H = \mathcal{H}_1 | H \in S) = \frac{W(\mathcal{H}_1)}{W_H(G_C)}.$$

In Sub Algorithm II, let x_k , $1 \leq k \leq t$, denote the indication function of acceptance or rejection in Step 6, that is, $x_k = 1$ if a Hamiltonian cycle is accepted and $x_k = 0$ otherwise. Obviously, x_k , $1 \leq k \leq t$, are i.i.d. Bernoulli random variables with $P(x_1 = 1) = p = W_H(G_C)/Br(C) = \text{ham}(C)/Br(C)$. Let A_G^ε be the matrix obtained in Step 1 of Sub Algorithm I. Hence, by Lemma 6 and noting $t = 4N(\varepsilon/2)^{-2} \log(\delta^{-1})$, where $N = Br(C)/\text{ham}(C)$, a simple calculation shows

$$P((1 - \varepsilon/2) \text{ham}(A_G^\varepsilon) \leq \widetilde{\text{ham}}(A_G) \leq (1 + \varepsilon/2) \text{ham}(A_G^\varepsilon)) \geq 1 - \delta.$$

Noting $\text{ham}(A_G) \leq \text{ham}(A_G^\varepsilon) \leq (1 + \varepsilon/3) \text{ham}(A_G)$, thus the proof completes. \square

4. Complexity and Hardness of Counting

4.1. Complexity of the Algorithm

Due to ellipsoid method[15], the running time of matrix scaling is $O(n^4 \log n)$. So the complexity of Sub Algorithm I is $O(n^4 \log n)$.

The time of repeating Step 6 in Sub Algorithm II is $t = O(\text{Br}(C)/\text{ham}(C))$, and for each time the running time is $O(n^2)$, hence, the complexity of Sub Algorithm II is $O(n^2 * t) = O(n^2 \text{Br}(C)/\text{ham}(C))$, where $\varepsilon^{-2} \log \delta^{-1}$ has been put into the term $O(\cdot)$ for simplicity. As we know, the Hamiltonian Recovery Algorithm takes $O(n^2)$ time. After removing Hamiltonian Recovery procedure, the total running time of Sub Algorithm II is still $O(n^2 * t)$, thus if approximating $\text{ham}(A_G)$ is only the purpose, outputting the Hamiltonian cycle is the byproduct of Sub Algorithm II.

If the digraph G is αn dense, $\alpha > .5$, an important result given by Huber[10] is

$$\text{Br}(C)/\text{per}(C) = O(n^{-.5+.5/(2\alpha-1)}).$$

Note that

$$\frac{\text{per}(C)}{\text{ham}(C)} = \frac{\prod_{i=1}^n (X(i,i)Y(i,i)Z(i,i)) \text{per}(A_G^\varepsilon)}{\prod_{i=1}^n (X(i,i)Y(i,i)Z(i,i)) \text{ham}(A_G^\varepsilon)} = \frac{\text{per}(A_G^\varepsilon)}{\text{ham}(A_G^\varepsilon)}.$$

If the digraph G is at least $.5n$ dense, then changing any zeros in A_G to εn^{-3} increases $\text{per}(A_G)$ by at most a factor of $1 + \varepsilon$ [11]. Then

$$\frac{\text{per}(C)}{\text{ham}(C)} = \frac{\text{per}(A_G^\varepsilon)}{\text{ham}(A_G^\varepsilon)} \leq \frac{(1 + \varepsilon/3) \text{per}(A_G)}{\text{ham}(A_G)} = O\left(\frac{\text{per}(A_G)}{\text{ham}(A_G)}\right).$$

Hence, the total running time of our algorithm is

$$\begin{aligned} O(n^4 \log n + n^2 \frac{\text{Br}(C)}{\text{ham}(C)}) &= O(n^4 \log n + n^2 \frac{\text{Br}(C)}{\text{per}(C)} \frac{\text{per}(C)}{\text{ham}(C)}) \\ &= O(n^4 \log n + n^{1.5+.5/(2\alpha-1)} \frac{\text{per}(A_G)}{\text{ham}(A_G)}). \end{aligned} \quad (1)$$

Now we present combinatorial argument on the bound of $\frac{\text{per}(A_G)}{\text{ham}(A_G)}$ (Recall A_G is a 0-1 matrix and all the edge weight of G equals one). The methodology is analogous

to the approach for undirected graphs given by Dyer et.al.[6].

Lemma 8. ([6]) *Let n be a natural number and β a positive number. Let $k_0 = \max(\lfloor \beta \log n \rfloor, 1)$ and $g(k) = n^\beta k! (\beta \log n)^{-k}$, define*

$$f(k) = \begin{cases} g(k), & k \leq k_0 \\ g(k_0), & k > k_0. \end{cases}$$

Then $f(k-1) \geq (\beta \log n) k^{-1} f(k)$; and $f(k) \geq 1$ for any k .

Proof. If $k \leq k_0$, $f(k-1) = g(k-1) = (\beta \log n) k^{-1} g(k) = (\beta \log n) k^{-1} f(k)$;

If $k > k_0$, then $\beta \log n / k \leq 1$. Hence

$$f(k-1) = g(k_0) \geq (\beta \log n) k^{-1} g(k_0) = (\beta \log n) k^{-1} f(k).$$

Thus $f(k) \geq f(k_0)$, we have

$$\frac{1}{f(k)} \leq \frac{1}{f(k_0)} \leq \frac{(\beta \log n)^{k_0}}{n^\beta (k_0)!} \leq n^{-\beta} \sum_{k=0}^{\infty} \frac{(\beta \log n)^k}{(k)!} \leq n^{-\beta} e^{\beta \log n} = 1. \quad \square$$

Theorem 9. *Suppose $\alpha \in (.75, 1]$. Let G be an αn dense digraph and F_k the set of 1-factors in G containing exactly k cycles, $1 \leq k \leq \lfloor n/2 \rfloor$. Note that F_1 is the set of Hamiltonian cycles in G . Let $F = \bigcup_k F_k$. Then*

$$\frac{|F|}{|F_1|} = O(n^{1+1/(2\alpha-1.5)}).$$

With this theorem, we prove the main result of this paper Theorem M.

Proof of Theorem M. By theorem 9, since $|F|/|F_1| = \text{per}(A_G)/\text{ham}(A_G)$, and noting (1), therefore Theorem M follows immediately.

Now we proceed to prove Theorem 9.

Proof of Theorem 9. We construct a new weighted digraph $\Psi = (F, K)$. K is defined as follows.

$$K = \{(E, E') : E \in F_k, E' \in F_{k'}, k' < k \text{ and } E \oplus E' \cong \overline{C_4}\},$$



Figure 1: The symmetric differences $\overline{C_4} = E \oplus E'$

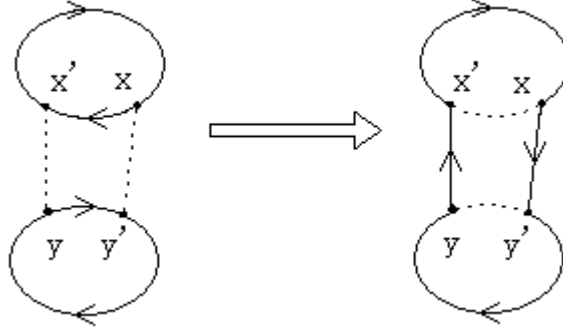


Figure 2: E' is obtained by coalescing two cycles of E into a single cycle

where $\overline{C_4}$ is a graph with four vertices and four edges, in which two vertices have indegrees two, outdegrees zero, and the other two vertices have indegrees zero, outdegrees two (See Figure 1). The four edges belong to E and E' alternatively. To avoid the confusion with vertices and edges in G , we call the *nodes* and *arcs* corresponding to F and K in Ψ . Observe also that if $(E, E') \in K$ is an arc of Ψ , E' can be obtained from E by deleting two edges and adding two others, and that this operation can decrease the number of cycles by one (See Figure 2). Hence every arc (E, E') is directed from a node E in some F_k to a node E' in F_{k-1} .

The proof strategy is to define a positive weight function w on the arcs set K such that the total weight of arcs leaving each node $E \in F/F_1$ is at least one greater than the total weight of arcs entering E . Denote $w^+(S)$ and $w^-(S)$ the total weight leaving and entering a node set S in Ψ respectively, the strategy ensures

$$w^-(F_k) + |F_k| = \sum_{E \in F_k} (w^-(E) + 1) \leq \sum_{E \in F_k} w^+(E) = w^+(F_k), \quad k \geq 2.$$

Hence,

$$w^-(F_1) = w^+(F_2) = \sum_{k \geq 2} (w^+(F_k) - w^-(F_k)) \geq \sum_{k \geq 2} |F_k| = |F/F_1|.$$

Let $g = \max_{E \in F_1} w^-(E)$. Since $w^-(F_1) = \sum_{E \in F_1} w^-(E) \leq g|F_1|$, then

$$|F|/|F_1| \leq g + 1.$$

The weight function $w : K \rightarrow \mathcal{R}^+$ defined as follows. For any arc (E, E') with $E' \in F_k$, we know E' is obtained by coalescing two cycles of E , and suppose the length of these two cycles are l_1 and l_2 , then define $w(E, E') = (l_1^{-1} + l_2^{-1})f(k)$, where $f(k)$ is defined as in Lemma 8. Then we have the following two claims.

Claim 1. For any $E \in F_k$, $k \geq 2$, $w^+(E) \geq (2\alpha - 1.5)n\beta f(k) \log n + 2$.

Claim 2. For any $E \in F_k$, $k \geq 1$, $w^-(E) \leq n \log n f(k)$.

By these two claims, set $\beta = 1/(2\alpha - 1.5)$. Then for $E \in F_k$, $k \geq 2$, we have $w^+(E) - w^-(E) \geq 2 \geq 1$ and $g = \max_{E \in F_1} w^-(E) \leq n \log n f(1) \leq (2\alpha - 1.5)n^{1+1/(2\alpha-1.5)}$. Hence $|F|/|F_1| \leq g + 1 = O(n^{1+1/(2\alpha-1.5)})$, which completes the proof. \square

Proof of Claim 1. Let $E \in F_k$ be an 1-factor with k cycles $\gamma_1, \dots, \gamma_k$, of lengths n_1, n_2, \dots, n_k , $k \geq 2$. We proceed to bound $w^+(E)$. To show the lower bound of $w^+(E)$, we need to count the number of arcs leaving E . Suppose (E, E') to be such an arc. Let $\gamma = E \oplus E'$, $E' \in F_{k-1}$, be the form (x, x', y, y') , where $(x, x'), (y, y') \in E$ and $(y, x'), (x, y') \in E'$.

First, we estimate the number of $\overline{C_4}$ -type cycles γ for which (x, x') is contained in a particular cycle $\gamma_i \in E$. We say that γ is *rooted* at γ_i . Assume, for a moment, that the vertices x, x' is chosen. There are at least $\alpha n - (n_i - 1)$ ways to extend the path first to y then to y' since the indegrees of x' is at least αn . Denote Y' the set of all vertices y' reachable. Recall $N^+(x, G)$ is the set of neighbors x points to. Thus the number of ways of completing a $\overline{C_4}$ -type cycle (x, x', y, y') is at least

$$\begin{aligned} |N^+(x, G)| + |Y'| - n &\leq \alpha n + (\alpha n - (n_i - 1)) - n \\ &= 2\alpha n - n_i - n + 1. \end{aligned}$$

Hence the total number of $\overline{C_4}$ -type cycles rooted at γ_i is at least $n_i(2\alpha n - n_i - n + 1)$.

We are now poised to bound $w^+(E)$. Each arc (E, E') defined by a $\overline{C_4}$ -type γ rooted at γ_i has weight at least $n_i^{-1}f(k-1)$, which, by Lemma 8, bounded below by $(\beta \log n)(kn_i)^{-1}f(k)$, Thus

$$\begin{aligned}
w^+(E) &= \sum_{E':(E,E') \in K} w(E, E') \\
&\geq \sum_{i=1}^k n_i(2\alpha n - n_i - n + 1)n_i^{-1}f(k-1) \\
&= \sum_{i=1}^k (2\alpha n - n_i - n)f(k-1) + kf(k-1) \\
&\geq (2\alpha kn - n - kn)(\beta \log n)k^{-1}f(k) + kf(k-1) \\
&= (2\alpha - 1/k - 1)(\beta \log n)f(k)n + kf(k-1) \\
&\geq (2\alpha - 1.5)(\beta \log n)f(k)n + 2.
\end{aligned}$$

For the first inequality, it seems we have overcounted the weight. we explain the reason. When (x, x') is rooted at γ_i and (y, y') lies in some γ_j if we extends (x, x') to (y, y') to complete a $\overline{C_4}$ -type cycle $\gamma = (x, x', y, y')$, the contribution to the weight is only $n_i^{-1}f(k-1)$ in the above inequality. Similarly, when (x, x') is rooted at the same position as (y, y') in γ_j and (y, y') lies in the same position as (x, x') in γ_i , the contribution to the weight is $n_j^{-1}f(k-1)$. Plus these two weight, $(n_j^{-1} + n_i^{-1})f(k-1)$ is exactly $w(E, E')$ needed to be considered by the definition of w , where $E \oplus E' = \gamma$. Hence, though each $\overline{C_4}$ cycle is counted twice, the weight not. The last inequality follows immediately from $k \geq 2$ and $f(k-1) \geq 1$. \square

Proof of Claim 2. For each $E \in F_k$, we now proceed to bound $w^-(E)$. Let (E', E) be an arc in K . It is straightforward to verify that the $\overline{C_4}$ -type $\gamma = (x, x', y, y') = E \oplus E'$ must contain two edges (x, x') and (y, y') from a single γ_i of E , and $(y, x'), (x, y') \in E'$. Removing these two edges from γ_i leaves a double of simple paths of lengths $p-1$ and $q-1$, where $p, q \geq 2$. For the case $p \neq q$ there are at most n_i ways such that $\gamma_i \oplus \gamma$ is a pair of cycles with length p and q , and $n_i/2$ ways such that $\gamma_i \oplus \gamma$ is a pair of cycles with length p and q for the case $p = q$. Noting both cases happen when γ_i is contained in a complete sub digraph of G or G is a complete digraph(Complete digraph is defined as such a digraph that any two distinct vertices have edges pointing to each other). Hence

$$\begin{aligned}
w^-(E) &= \sum_{E':(E',E) \in K} w(E', E) \\
&\leq \sum_{i=1}^k n_i f(k) \sum_{\substack{p>q \geq 2 \\ p+q=n_i}} \left(\frac{1}{p} + \frac{1}{q}\right) + \frac{1}{2} \sum_{i=1}^k n_i f(k) \sum_{\substack{p=q \geq 2 \\ p+q=n_i}} \left(\frac{1}{p} + \frac{1}{q}\right) \\
&\leq \frac{1}{2} \sum_{i=1}^k n_i f(k) \sum_{\substack{p,q \geq 2 \\ p+q=n_i}} \left(\frac{1}{p} + \frac{1}{q}\right) \\
&= \frac{1}{2} \sum_{i=1}^k n_i f(k) \sum_{p=2}^{n_i-2} \left(\frac{1}{p} + \frac{1}{n_i-p}\right) \\
&= \sum_{i=1}^k n_i f(k) \sum_{p=2}^{n_i-2} \left(\frac{1}{p}\right) \\
&\leq \sum_{i=1}^k n_i f(k) \log n_i \\
&\leq n \log n f(k). \quad \square
\end{aligned}$$

4.2. Hardness of Counting Hamiltonian cycles in dense digraphs

We first declare the notation related to undirected graphs only appears in this subsection and the notation related to digraph is the same as that in the previous sections. Our reduction comes from the undirected graph, hence notation for undirected graphs is needed. Let G be a simple *undirected* graph with vertices $\{1, 2, \dots, n\}$, where $n \geq 3$. The definition of a Hamiltonian cycle of an undirected graph is a closed undirected path that visits each vertex once and only once. We use the notation $m_1 m_2 \dots m_n m_1$ to denote a Hamiltonian cycle in an undirected graph (recall $(m_1, m_2, \dots, m_n, m_1)$ denotes a Hamiltonian cycle in digraphs). The degree of a vertex in an undirected graph G is defined as the number of its neighbors. Let $\#HC$ and $\#DHC$ be the problem of counting the number of Hamiltonian cycles in undirected and directed graphs respectively. Now define a symmetric digraph G' corresponding to an undirected graph G by replacing each edge (i, j) of G with two directed edges (i, j) and (j, i) . Let H_G and $H_{G'}$ denote the set of the Hamiltonian cycles in G and G' respectively. Let $\mathcal{P}(H_{G'})$ denote the power set of $H_{G'}$. We will prove the number of Hamiltonian cycles in an undirected graphs equals half of the

number of Hamiltonian cycles in its corresponding symmetric digraphs.

Lemma 10. ([6]) *#HC is #P-Complete, even when restricted to graphs G of minimum degree at least $(1 - \varepsilon)n$, for any $\varepsilon > 0$*

Lemma 11. *Let $\mathcal{H} = m_1 \cdots m_n m_1$ be a Hamiltonian cycle in H_G . Then there are at least two Hamiltonian cycles (m_1, \dots, m_n, m_1) and (m_1, m_n, \dots, m_1) in $H_{G'}$. Define a map φ from H_G to $\mathcal{P}(H_{G'})$ as follows:*

$$\varphi(\mathcal{H}) = \{(m_1, \dots, m_n, m_1), (m_1, m_n, \dots, m_1)\}.$$

Let $Im\varphi$ denote the image set of the map φ , and let $\mathcal{H}' = m'_1 \cdots m'_n m'_1$ be a different Hamiltonian cycle from \mathcal{H} in H_G . Then

$$\varphi(\mathcal{H}) \cap \varphi(\mathcal{H}') = \emptyset \quad \text{and} \quad \cup Im\varphi = H_{G'}.$$

Proof. Due to the symmetry of the digraph G' , and noting $n \geq 3$, for any Hamiltonian cycle (m_1, \dots, m_n, m_1) in $H_{G'}$, there must be a different Hamiltonian cycle (m_1, m_n, \dots, m_1) in $H_{G'}$. These two Hamiltonian cycles obviously has a pre-image, the Hamiltonian cycle $m_1 \cdots m_n m_1$ in H_G . Note (m_1, \dots, m_n, m_1) is in $\varphi(m_1 \cdots m_n m_1)$. Hence, $\cup Im\varphi \supseteq H_{G'}$. Obviously, $\cup Im\varphi \subseteq H_{G'}$. Therefore

$$\cup Im\varphi = H_{G'}.$$

Suppose there are two different Hamiltonian cycles $\mathcal{H} = m_1 \cdots m_n m_1$ and $\mathcal{H}' = m'_1 \cdots m'_n m'_1$ in H_G . Let $N_{\mathcal{H}}(m_i)$ denote two neighbor vertices of vertex m_i in \mathcal{H} . \mathcal{H} and \mathcal{H}' are different if and only if there exists a vertex $\{m_i\} = \{m'_j\}$ such that $N_{\mathcal{H}}(m_i) \neq N_{\mathcal{H}'}(m'_j)$. Hence (m_1, \dots, m_n, m_1) is different from $(m'_1, \dots, m'_n, m'_1)$ and $(m'_1, m'_n, \dots, m'_2, m'_1)$, that is $(m_1, \dots, m_n, m_1) \notin \varphi(\mathcal{H}')$. Similarly, $(m_1, m_n, \dots, m_1) \notin \varphi(\mathcal{H}')$. Hence $\varphi(\mathcal{H}) \cap \varphi(\mathcal{H}') = \emptyset$. \square

Theorem 12. *#DHC is #P-Complete, even when the digraph is $(1 - \gamma)n$ dense, $0 < \gamma < .5$.*

Proof. Lemma 11 shows the number of Hamiltonian cycles in an undirected graph is half of the number of Hamiltonian cycles in its corresponding symmetric digraph. Hence by Lemma 10, #DHC in $(1 - \gamma)n$ dense digraphs is #P-Complete, for any $0 < \gamma < .5$. \square

5. Conclusions and Discussions

The results in this paper show that for relatively dense digraphs, approximating the number of Hamiltonian cycles or generating weighted Hamiltonian cycles exactly from their correct distribution can be accomplished in $O(n^{2.5+.5/(2\alpha-1)+2/(4\alpha-3)})$ time. This is an improvement in running time by a factor of $n^{4.5}(\log n)^4$ for $.85n$ dense digraphs. Counting the number of Hamiltonian cycles in such digraphs is shown to be #P-Complete.

Estimating the Hamilton of a 0-1 matrix to within a factor of $1 + \varepsilon$ with probability at least $1 - \delta$, the running time is

$$O(n^{2.5+.5/(2\alpha-1)+1/(2\alpha-1.5)}\varepsilon^{-2}\log(\delta^{-1})).$$

It is known [2] that $0.5n$ dense digraphs contain Hamiltonian cycles. Our algorithm presented in this paper is shown to be an FPRAS for $0.75n$ dense problems. Hence a gap still remains. We can extend the definition $\overline{C_4}$ in the proof of Theorem 9, as shown by Figure 1. Similarly that can also be done to $\overline{C_6}$, $\overline{C_8}$. However it seems unlikely to obtain any better bounds than that by $\overline{C_4}$ in this way. This gap is left open here.

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